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ADP012802

TITLE: Hierarchy of Effective-Mass Equations for Semiconductor Nanostructures

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TITLE: Nanostructures: Physics and Technology International Symposium [6th] held in St. Petersburg, Russia on June 22-26, 1998 Proceedings

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ADP012712 thru ADP012852

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Hierarchy of effective-mass equations for semiconductor nanostructures

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Abstract. It has been developed a generalization of the Kohn–Luttinger envelope-function method that is applicable for description of the electron and hole states in many-layer (001) heterostructures, composed of related lattice-matched III–V semiconductors, with atomically abrupt heterointerfaces. It was shown that additional contributions to the standard one-band effective-mass equations may be classified with powers of the parameter $\bar{k}a_{\max} \ll 1$, where $1/\bar{k}$ is the characteristic size of the envelope function, and the length a_{\max} is of the order of the lattice constant. It was formulated a hierarchy scheme for the effective-mass equations, the n th level of which accounts for taking into consideration all corrections up to $(\bar{k}a_{\max})^n$. Zero level of the hierarchy corresponds to the standard effective-mass equations with position-independent effective mass. On the first level of the hierarchy each heterointerface gives an additional δ -function contribution to the potential energy. Only on the second level the position-dependent effective mass appears as well as corrections for the weak non-parabolicity of the spectrum and spin-orbit interface interaction. At higher levels of the hierarchy non-local contributions appear, and a one-band differential effective-mass equation does not exist.

Currently the question on applicability of the envelope-function (EF) method of Luttinger and Kohn [1] and the effective-mass (EM) equations for real nanostructures is discussed intensively [2]. There are several problems associated with the envelope-function method for heterostructures. The first one is whether the method can really be applicable when studied are the structures whose potential changes considerably on the lattice constant scale. As the matter of fact to researchers' attention the question has been overtopped with the second problem concerning the correct form of the effective kinetic energy operator (KEO) in the effective-mass method, which is just the one-band EF approximation, when EM parameters are position-dependent. To avoid this second problem some authors prefer using complicated many-band EF schemes even when the simple one-band approximation would provide them with at least qualitatively correct solution. Eliminating the KEO problem this way one still has a trouble with the first question. The main goal of the work is to derive simple EM equations for heterostructures taking into account abruptness of the heterostructure potential as well as position-dependent EM. Considered are the (001) heterostructures composed of related (band offsets are small as compared to the band gaps) lattice-matched III–V semiconductors. The presented below result is a kind of recipe, but the recipe based on a rigorous formalism of the Luttinger–Kohn EF method [2].

Generally, one-band EF equations (an equation for simple band and a set of equations for degenerate band) are obtained via a perturbation theory procedure. So there must be small parameters. When one deals with shallow states, the typical energy of which \bar{E} is small as compared to the typical energy separation from other bands \bar{E}_g , such a small parameter is $\sqrt{\bar{E}/\bar{E}_g}$. The small parameter may be put down as $\lambda\bar{k}$; here \bar{k} is

the characteristic wave number of the state in question, and $\lambda = 2\hbar\bar{P}/(m_0\bar{E}_g)$, where \bar{P} is the typical interband matrix element of momentum and m_0 is the free electron mass. When the proper band edge EM m is mainly formed with the $\mathbf{k} \cdot \mathbf{p}$ interaction, we may adopt $\lambda \sim \hbar/\sqrt{m\bar{E}_g}$. Another small parameter emerges when we face abrupt changes of the heterostructure potential. The parameter is $a\bar{k}$, where a is the lattice constant. It is important that for a good deal of materials we have $a \sim \lambda$ (e.g. for GaAs $\lambda \approx 6 \text{ \AA}$). This is the reason why we should retain terms to the same order in these two parameters in the one-band EF equations. Now we are about to discuss the obtained EM equations. The equations are presented the way they govern electron and hole states in a (001) symmetric quantum well of width L in the absence of external potentials, and $L = \mathcal{N}a/2$, where \mathcal{N} is an integer.

In the usual (bulk) EM equation [1] for electrons

$$[\hat{T} + V(z)] F_c = EF_c,$$

the KEO and potential energy have standard form:

$$\hat{T}_{\text{bulk}} = \frac{\mathbf{p}^2}{2m}; \quad V_{\text{bulk}}(z) = \Delta E_c \{\Theta(-z) + \Theta(z-L)\}, \quad (1)$$

where m is the bulk EM, ΔE_c is the conduction band offset, F_c is the conduction band EF. The function V_{bulk} describes the rectangular shape of the conduction band QW. Allowing for $\mathbf{k} \cdot \mathbf{p}$ interaction with remote bands as well as terms arisen due to abrupt change of the potential at the heterointerfaces give an opportunity to classify these contributions with powers of the parameter $\bar{k}a_{\text{max}} \ll 1$, where $a_{\text{max}} = \max(\lambda, a)$. We present the hierarchy scheme for the EM equations, where the n th level of the hierarchy accounts for taking into consideration all corrections up to $(\bar{k}a_{\text{max}})^n$.

Conduction band QW states near Γ point

0e) Zero level of the hierarchy for electrons. The effective Hamiltonian has “bulk” form (1), that is

$$\hat{T}^{(0)} = \hat{T}_{\text{bulk}}; \quad V^{(0)}(z) = V_{\text{bulk}}(z).$$

We emphasize that at this (the main!) level of the hierarchy $m(z) = \text{const}$.

1e) First level of the hierarchy. As taken into account are terms having $a\bar{k}$ smallness, KEO does not change, and in the potential energy there appear δ -function corrections:

$$\hat{T}^{(1)} = \hat{T}_{\text{bulk}}; \quad V^{(1)}(z) = V_{\text{bulk}}(z) + d_1 \{\delta(z) + \delta(z-L)\}.$$

The appearance of the two δ -functions at the heterointerfaces is due to abrupt change of the potential and corrections arisen as we describe the real (non-abrupt) form of the heterostructure potential with the Heaviside step-functions. The parameter d_1 depends both on bulk properties of the structure components and the microscopic form of the transition region of the heterojunction (HJ), and generally differs for each different heterointerface.

2e) Second level of the hierarchy. If we wish to take into account corrections of the order of $(a\bar{k})^2$, $(\lambda\bar{k})^2$ and $(a\bar{k})(\lambda\bar{k})$, we should deal with the equation where the concept of the position-dependent EM appears:

$$\hat{T}^{(2)} = \frac{1}{2} m^\alpha(z) \mathbf{p} m^\beta(z) \mathbf{p} m^\alpha(z) + \alpha_0 \mathbf{p}^4 + \beta_0 (\mathbf{p}_x^2 \mathbf{p}_y^2 + \mathbf{p}_x^2 \mathbf{p}_z^2 + \mathbf{p}_y^2 \mathbf{p}_z^2);$$

$$V^{(2)} = V^{(1)} + d_2 [\mathbf{p} \times \mathbf{n}] \cdot \sigma \{ \delta(z) - \delta(z-L) \}$$

Here $m(z)$ is the position-dependent band edge EM, α_0 and β_0 are the weak non-parabolicity parameters, \mathbf{n} is the unit Oz -axis vector, σ are the Pauli matrices. The parameters α (for β we have $2\alpha + \beta = -1$) and d_2 also depend on bulk properties of the materials of the structure as well as on the microscopic structure of the heterointerface, and should be different for each different HJ (we have a symmetric structure, so the parameters are the same for both HJs). The parameter d_2 originates from spin-orbit interaction, which is taken into account through the perturbation theory, the typical spin-orbit interaction parameter being considered to be of the order of the band offsets (the case takes place for a good deal of heterostructures).

Now we present the reasons why one cannot achieve better accuracy for the one-band approximation in the framework of differential equations of finite order. Originally the many-band set of $\mathbf{k} \cdot \mathbf{p}$ equations is a set of \mathbf{k} -space integral equations, and \mathbf{k} -space is restricted with the first Brillouin zone. For shallow states one may use an approximate canonical transformation of the set (or another unitary perturbation scheme) and move onto the one-band EF approximation. It is important that not all \mathbf{k} belonging to the first Brillouin zone may now correctly contribute to such an equation. The evidence comes from the following. For a bulk material one may use a series to present the spectrum $\epsilon(\mathbf{k})$ of the states near Γ point. Such a series has a finite radius of convergence K_0 , which is determined with the strength of the $\mathbf{k} \cdot \mathbf{p}$ interaction and proximity of other bands. The estimation gives $K_0 \sim 1/\lambda$. This way for the one-band EF equation \mathbf{k} -space is restricted with radius K_0 rather than the first Brillouin zone boundary. To obtain differential equations in \mathbf{r} -space one should go beyond the \mathbf{k} -space effective limits. The procedure would induce an exponentially small error if either potential or EF were smooth on the lattice constant scale. That would mean the Fourier transform of either potential or EF drops exponentially as \mathbf{k} increases. But in our case we have abrupt heterostructure potential. One may see from all above that F_c is not smooth, in particular its second derivative has two discontinuities with the relative jumps of the order of unit. This means that if L is large enough, e.g. the conduction band EF Fourier transform $\mathcal{F}_c(\mathbf{k}) \propto 1/(k_z)^3$. So, the principal error of the one-band method is $(\bar{k}/K_0)^3 \sim (\lambda\bar{k})^3$. It is the error that does not allow one to reach better accuracy than that given with the second level equation.

Hole QW states near Γ point

The only difference between the EM method for conduction and valence bands lies in more complicated character of the EF equations for the latter case. This way zero hierarchy level of accuracy of the one-band EM method is plain. As for the second one, the proper equation has so many parameters, some of which depend on specific microscopic details of heterointerfaces, that in practice it would be useless, and similar equation for simple band could have probably satisfied the academic interest. So, we present the first grade. In this approximation the Hamiltonian for valence band states is a sum of the standard (bulk) 6×6 KEO matrix, and the potential energy 6×6 matrix. It is the latter that is presented below. We use the basis $\{|J, j_z\rangle\}$ of eigenfunctions of the total angular momentum J and his projection j_z , which are linear combinations of

the Γ_{15} valence band edge Bloch functions and spin. We adopt the following ordering:

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle, \quad \left| \frac{3}{2}, -\frac{3}{2} \right\rangle, \quad \left| \frac{3}{2}, \frac{1}{2} \right\rangle, \quad \left| \frac{3}{2}, -\frac{1}{2} \right\rangle, \quad \left| \frac{1}{2}, \frac{1}{2} \right\rangle, \quad \left| \frac{1}{2}, -\frac{1}{2} \right\rangle,$$

and the phase agreement is the same as in [1]. So, the potential energy matrix is

$$\mathbf{V} = \begin{pmatrix} V_{\Gamma_8} \mathbf{1} & V_0 \sigma_y & -i\sqrt{2}V_0 \sigma_y \\ V_0^\dagger \sigma_y & V_{\Gamma_8} \mathbf{1} & \mathbf{0} \\ i\sqrt{2}V_0^\dagger \sigma_y & \mathbf{0} & V_{\Gamma_7} \mathbf{1} \end{pmatrix}. \quad (2)$$

Here

$$V_{\Gamma_8} = E_{\Gamma_8} + \Delta U_{\Gamma_8} \{ \Theta(-z) + \Theta(z-L) \} + \chi_1 \{ \delta(z) + \delta(z-L) \},$$

$$V_{\Gamma_7} = E_{\Gamma_7} + \Delta U_{\Gamma_7} \{ \Theta(-z) + \Theta(z-L) \} + \chi_2 \{ \delta(z) + \delta(z-L) \},$$

$$V_0 = \chi_3 \{ \delta(z) - \delta(z-L) \}.$$

The notations are the following: E_{Γ_8} and E_{Γ_7} are the Γ_8 and Γ_7 band edge energies of the well material, ΔU_{Γ_8} and ΔU_{Γ_7} are the proper band offsets. Two parameters χ_1 and χ_2 have the same origin as d_1 for the conduction band case, and the parameter χ_3 appears only as we correctly process the abrupt changes of the heterostructure potential (that means the parameter vanishes for smooth potentials). The last parameter defines in particular the strength of the zone center mixing of light and heavy holes [3].

In conclusion we presented three grades of accuracy that can be achieved in the one-band EF approximation, and this way formulated three hierarchy levels for the EM equations. There are effects that cannot be described using the zero level of the hierarchy, e.g. zone center light hole-heavy hole mixing in the valence band. There are also effects that can be dealt with only using the second-level equations of the hierarchy, e.g. spin splitting of the subbands when longitudinal electric field is applied (when the presence of the terms like the one proportional to d_2 is crucial), or some optical transitions.

The work was supported by RFBR (project 96-02-18811), RFBR-INTAS (95-0849), the Federal Programs “Physics of Solid State Nanostructures” (96-1019), and “Surface Atomic Structures” (95-3.1).

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